

Comment on “ \mathbb{Z}_2 spin liquid phase on the kagome lattice: a new saddle point”, by Tao Li [arXiv:1601.02165 (2016)]

In a recent paper, Tao Li [1] claimed that a gapped \mathbb{Z}_2 spin liquid, obtained using projected Gutzwiller fermionic wave functions, can be stabilized in the Heisenberg model on the kagome lattice. According to his calculations, the best wave function is gauge equivalent to the so-called $\mathbb{Z}_2[0, \pi]\beta$ state that has been proposed in Ref. [2] and numerically studied by us [3]. The major claim was that the \mathbb{Z}_2 state has a (slightly) lower energy than its “parent” $U(1)$ Dirac spin liquid, which is recovered once the spinon pairing is switched off. Calculations were done for the Heisenberg model with nearest-neighbor (NN) J_1 and next-nearest-neighbor (NNN) J_2 super-exchange couplings. The energy gain was claimed to be “substantial” for $J_2/J_1 = 0.15$, but also finite for $J_2 = 0$. However, the values of the energy gain were reported only in few cases, without performing a size scaling (numbers for $J_2 = 0$ were not reported), while the size scaling for some variational parameters have been shown for $J_2/J_1 = 0.15$.

In this comment, we perform very accurate variational calculations with both $U(1)$ and \mathbb{Z}_2 wave functions, with much smaller error bars with respect to our recent calculations [4], and show that even though a small energy gain is found (compatible with our previous results), it goes to zero when increasing the size of the cluster, as already claimed in our previous work [4]. We thus confirm with unprecedented accuracy the fact, that the \mathbb{Z}_2 spin liquid is a local energy minimum that goes away with system size. Therefore, our calculations confirm once more that the $U(1)$ spin liquid with Dirac nodes is stable against the opening of a spin gap, not only for $J_2 = 0$, but also for small values of J_2/J_1 , e.g., $J_2/J_1 = 0.15$.

The variational wave function for the spin model is obtained by applying the Gutzwiller projector \mathcal{P}_G to an uncorrelated wave function:

$$|\Psi_{\text{var}}\rangle = \mathcal{P}_G|\Phi_0\rangle, \quad (1)$$

where $|\Phi_0\rangle$ is the ground state of a BCS Hamiltonian that contains NN real hopping (χ_1 , which can be taken as the energy scale, i.e., $\chi_1 = 1$), NNN real hopping (χ_2) and spinon pairing (Δ_2), and two on-site terms, one for the chemical potential (μ) and the other for the real on-site pairing (ζ_R). A non-trivial sign structure for the hopping and pairing terms is assumed [2, 3], e.g., a fictitious gauge magnetic flux is piercing each unit cell. The $U(1)$ Dirac state is obtained by taking $\Delta_2 = 0$ and $\zeta_R = 0$ (in this case the chemical potential is irrelevant, not changing the single-particle orbitals).

Our results are summarized in Table I and Fig. 1. Here, we optimized χ_2 for the $U(1)$ state, while we used the variational parameters obtained in Refs. [1, 5] for the \mathbb{Z}_2 wave function and computed the energies of the gapless $U(1)$ and gapped \mathbb{Z}_2 states. Although

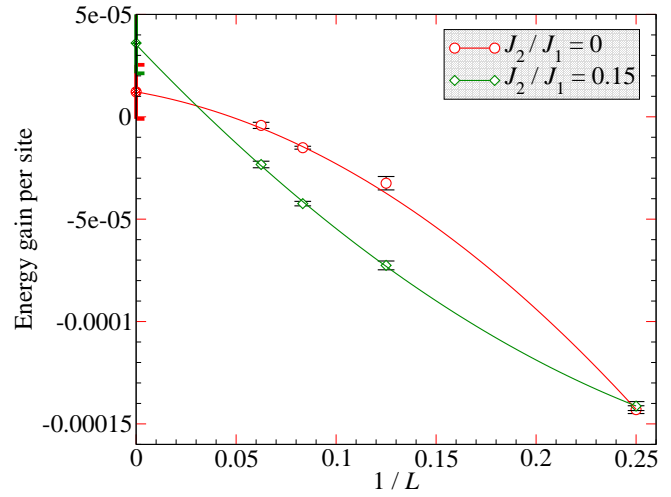


FIG. 1. The size scaling of the energy gain per site $\Delta E = E_{\mathbb{Z}_2} - E_{U(1)}$ is shown for $J_2 = 0$ and $J_2/J_1 = 0.15$, for $L = 4, 8, 12$ and 16 clusters. The results for $L = 4$ and 8 are from Ref. [4].

the gapped spin liquid has a slightly lower energy than the gapless one, namely $\Delta E = -0.0000044(13)$ for $J_2 = 0$ and $-0.0000226(14)$ for $J_2/J_1 = 0.15$ on the 768-site cluster, the size scaling clearly show that, in the thermodynamic limit, the \mathbb{Z}_2 Ansatz does not give a finite energy gain. Indeed, for $J_2/J_1 = 0$, the gain is zero within the errorbars, and for $J_2/J_1 = 0.15$, it is zero within two errorbars. Hence, the fact that the energy gain of the gapped $\mathbb{Z}_2[0, \pi]\beta$ spin liquid goes to zero in the thermodynamic limit is *irrefutable*.

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 - [5] T. Li, private communication.

J_2/J_1	$12 \times 12 \times 3 = 432\text{-site cluster}$			$16 \times 16 \times 3 = 768\text{-site cluster}$		
	$E_{U(1)}$	$E_{\mathbb{Z}_2}$	ΔE	$E_{U(1)}$	$E_{\mathbb{Z}_2}$	ΔE
0	-0.4287114(3)	-0.4287266(4)	-0.0000151(7)	-0.4287160(6)	-0.4287204(7)	-0.0000044(13)
0.15	-0.4346363(4)	-0.4346787(6)	-0.0000424(11)	-0.4347006(7)	-0.4347232(7)	-0.0000226(14)

TABLE I. Ground state energies per site (in units of J_1) of the $U(1)$ Dirac state (current work) and the $\mathbb{Z}_2[0, \pi]\beta$ state (Refs. [1, 5]) together with the energy gain per site ($\Delta E = E_{\mathbb{Z}_2} - E_{U(1)}$). The corresponding parameters are given in Table II.

J_2/J_1	$12 \times 12 \times 3 = 432\text{-site cluster}$				
	$U(1)$		\mathbb{Z}_2		
	χ_2	Δ_2	χ_2	μ	ζ_R
0	-0.019010(2)	-0.04147	-0.02294	-0.95615	-0.14969
0.15	0.154215(6)	-0.11783	0.14001	-0.29534	-0.33552

J_2/J_1	$16 \times 16 \times 3 = 768\text{-site cluster}$				
	$U(1)$		\mathbb{Z}_2		
	χ_2	Δ_2	χ_2	μ	ζ_R
0	-0.019522(3)	-0.03646	-0.02103	-0.90133	-0.14296
0.15	0.153695(4)	-0.11826	0.14187	-0.29038	-0.33811

TABLE II. Optimized parameters of the extended $U(1)$ Dirac SL (current work) and the $\mathbb{Z}_2[0, \pi]\beta$ state (corresponding to Refs. [1, 5]). The NN hopping is $\chi_1 = 1$. The corresponding energies are given in Table I.